Resonating Valence Bond Theory of Superconductivity for Dopant Carriers: Application to the Cobaltates

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Within the t–J model Hamiltonian we present a RVB mean field theory directly in terms of dopant particles. We apply this theory to $Na_x CoO_2 \cdot y H_2 0$ and show that the resulting phase diagram T_c versus doping is in qualitative agreement with the experimental results.

I.   INTRODUCTION

The remarkable discovery of superconductivity in $Na_x CoO_2 \cdot y H_2 0$ for $x = 0.35$ and $y = 1.30$ by Takada *et al.*[1] attracted a lot of attention. The experimental findings indicate several striking similarities between the cobaltates and the cuprates. $Na_x CoO_2 \cdot y H_2 0$ can be viewed as a $2D$ Mott insulator. The Co atoms form a triangular lattice but Co^{4+} is in a $s = \frac{1}{2}$ low spin state. The transition temperature (T_c) is seen to decrease for both underdoped and overdoped materials[2] although for the cobaltates the maximum T_c is much lower $(T_c \approx 5K)$ and the optimal doping is twice as large as in the cuprates. Finally, as one varies temperature and electron concentration, apart from superconductivity, there are observed unusual electronic properties[3] and clear hints that strong electronic correlation is at work in both cases.

All this turns attractive the application of the resonating valence bond (RVB) ideas to this new compound. Baskaran[4] was the first to present qualitative arguments in favor of the RVB approach for the cobaltates. Soon after that Kumar and Shastry[5] as well as Lee and coworkers[6,7] presented their first estimates for the mean field (MF) phase diagram, T_c versus doping, in a RVB framework. In the cobaltates the CoO_2 layers are arranged in a triangular lattice which naturally exhibits considerable magnetic frustration. This not only brings modifications to the symmetry of the resulting superconducting state, as pointed out by others,[4,5,6,7,8] but makes the the application of a MF RVB, to reproduce the experimental findings related to the superconductivity of $Na_x CoO_2 \cdot y H_2 0$, even more challenging. The reasons for that are as follows. The maximum T_c for the CoO_2 layers occurs for doping values nearly twice as large as in the cuprates. This might be indicative that the phase fluctuations of the superconducting (SC) order parameter could be much too strong for the stability of the MF RVB state. Moreover, in the standard approach low doping is always favored and makes even harder a more

quantitative agreement with experiment in the case of the cobaltates.

Within the original Baskaran-Zou-Anderson (BZA) MF approximation[9] a non-zero value of the RVB MF order parameter (OP) does not by itself imply superconductivity. The true SC OP in their approach is essentially taken as a product of a spinon (a spin-1/2 neutral fermion) pairing OP and a bose condensation factor for the holons (spin-0 charged bosons),[10] following the more conventional slave-boson approximation. The phase of the OP accounts for the fluctuations which drives T_c to zero at zero doping. The bose condensation temperature for the holons is estimated separately and the region in which both the spin-pairing OP and the mentioned holon bose factor are non-zero determines the resulting RVB superconducting phase.[5] All this seems to indicate that the standard MF RVB basic ingredients – the lattice spin singlet pairs – which might indeed be appropriate to describe the physics at very low dopings is not the best starting point to address the superconducting regime at higher doping values.

To overcome those limitations we present a RVB MF scheme which takes direct account of the dopant particles themselves and treats the non-double occupancy (NDO) constraint beyond the conventional slave-boson mean field approximation. As will be demonstrated by this and later works this RVB representation is most suitable to deal with cases in which strongly correlated electronic superconductivity is manifest in both low and high doping regimes.

In this first work we apply our method to the CoO_2 superconductors. Our starting point is the t-J model on a triangular lattice. In doing that we follow the arguments which consider the $3d$ levels of the Co^{4+} ions being crystal field split in the CoO_2 layers producing singly occupied non-degenerate spin-1/2 d_{z^2} orbitals. Those orbitals are directly associated with the singlet states in our t-J model representation based on the Hubbard X operators. The use of that representation will allow us to

go beyond the conventional treatment of the NDO constraint. The X operators are later given in a convenient coherent-state path-integral representation. The resulting variables in this representation are naturally split into bosonic and fermionic degrees of freedom. The bosonic modes correspond to SU(2) spin excitations while the fermion variables are spinless and describe U(1) charge excitations instead. Combining those spinon amplitudes and spinless fermion parameters together we then construct appropriate fermionic fields which carry both spin and charge degrees of freedom and can be directly related to the dopant carriers in the t-J model. We are able in this way to take a direct account of the doping dependence of the critical superconducting temperature preserving all the symmetry properties of the t-J Hamiltonian.

We reformulate the RVB theory of the SC phase entirely in terms of those quasiparticle states and use this scheme initially to describe the superconducting properties of the cobaltates. We find qualitatively good agreement with experiment and we are able to reproduce the observed dome structure of the T_c versus doping phase diagram for those materials in a RVB MF framework. The application of our RVB method to the cuprates will be presented in a subsequent work.

II. t-J HAMILTONIAN AND THE NDO CONSTRAINT

We start by expressing the t-J Hamiltonian[11]

$$H_{t-J} = -t \sum_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} + h.c. + J \sum_{ij} \left(\overrightarrow{Q}_i \overrightarrow{Q}_j - \frac{1}{4} n_i n_j \right),$$
(1)

with the NDO constraint, $\sum_\sigma n_{i\sigma} \leq 1$, in terms of the Hubbard operators,[12]

$$X_i^{\sigma 0} = c_{i\sigma}^+ \left(1 - n_{i-\sigma} \right), \quad n_{i-\sigma} n_{i\sigma} = 0.$$

Here $c_{i\sigma}$ is the electron annihilation operator at site i with the spin projection $\sigma = \uparrow\downarrow$, $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$, and the $\overrightarrow{Q}$'s are the corresponding electron spin operators. In terms of these operators the local NDO constraint holds rigorously and the t-J model becomes

$$H_{t-J} = -t \sum_{ij\sigma} X_i^{\sigma 0} X_j^{0\sigma} + h.c. + J \sum_{ij} \left(\overrightarrow{Q}_i \overrightarrow{Q}_j - \frac{1}{4} n_i n_j \right),$$
(2)

where the electron spin operator now reads $\overrightarrow{Q}_i = \frac{1}{2} \sum_{\sigma\sigma'} X_i^{\sigma 0} \overrightarrow{\tau}_{\sigma\sigma'} X_i^{0\sigma'}$, with the $\overrightarrow{\tau}$'s being Pauli matrices.

Fermionic operators $X_i^{\sigma 0}$ project the electron creation operators onto a space spanned by the basis $\{|0\rangle_i, |\sigma\rangle_i\}$ and take the form $X_i^{\sigma 0} = |\sigma\rangle_i \langle 0|_i$. Together with the bosonic generators, $X_i^{\sigma\sigma'} = |\sigma\rangle_i \langle \sigma'|_i$ the full set of operators X_i^{ab}, $a, b = 0, \uparrow, \downarrow$ forms, on every lattice site, a

basis of the fundamental representation of the semisimple doubly graded Lie algebra su(2|1) given by the (anti)commutation relations

$$\{X_i^{ab}, X_j^{cd}\}_\pm = (X_i^{ad}\delta^{bc} \pm X_j^{bc}\delta^{ad})\delta^{ij},$$

where the $(+)$ sign should be used only when both operators are fermionic.

Since su(2|1) can be viewed as a supergeneralization of the conventional spin su(2) algebra, the t-J Hamiltonian appears as a superextension of the Heisenberg magnetic Hamiltonian, with a hole being a superpartner of a su(2) magnetic excitation.[13] This superalgebra can also be thought of as a natural generalization of the standard fermionic algebra spanned by generators c_σ^+, c_σ, and unity I, to the case where the fermionic operators are subject to the NDO constraint. The incorporation of this constraint manifests itself in more complicated commutation relations between X operators in comparison with those produced by the conventional fermionic operators. Note that the Gutzwiller projection $P_G = \prod_i (1 - n_{i\sigma} n_{i-\sigma})$ that excludes the doubly occupied state $|\uparrow\downarrow\rangle$ is equivalent to the Hubbard operator representation, since $P_G c_{i\sigma}^+ c_{j\sigma} P_G = X_i^{\sigma 0} X_j^{0\sigma}$.

Note also that the occupation constraint is different for the hole and electron doping. To treat them in a unique way we perform, for electron dopings, a canonical particle-hole transformation $c_{i\sigma} \rightarrow c_{i-\sigma}^+$ that restores the non-double occupancy constraint but reverses the sign of t. Using then the Hubbard operator representation in terms of the transformed c-operators we again arrive at Eq.(2) with, however, $t \rightarrow -t$. Although the CoO$_2$ layer is an electron doped Mott insulator we shall for convenience formally deal with the more familiar case of hole doping making the necessary changes only at the end of our work.

Since the X operators are generators of the su(2|1) superalgebra we are lead naturally to employ the su(2|1) coherent-state path-integral representation of the t-J partition function. There are a few rationales to do that. First, this provides a mathematical setting well adjusted to address the t-J model with the crucial NDO constraint naturally built in the formalism from the very beginning. Second, within the su(2|1) path-integral representation the associated effective t-J action lives on a natural classical phase space of the t-J model – the SU(2|1) homogeneous compact manifold, $\text{CP}^{1|1}$ (see below). The group SU(2|1) acts on the $\text{CP}^{1|1}$ manifold as a group of canonical transformations in a way that the transformation properties of the basic fields – the local coordinates on $\text{CP}^{1|1}$ – can be easily found. Third, these coordinates are naturally split into bosonic and fermionic degrees of freedom. In the context of the t-J model the bosonic fields correspond to the SU(2) spin excitations whereas the fermionic ones are spinless and may be used to describe the U(1) charge excitations. This provides a natural setting to implement the spin-charge separation inherent in the spin liquid phase at least in 1D. Finally, the transformation properties of the $\text{CP}^{1|1}$ coordinates un-

der global SU(2)× U(1) rotations – the exact symmetry of the t-J Hamiltonian – imply that their certain combinations transform in the linear spinor representations of SU(2) and may therefore be used to describe fermionic quasiparticle excitations that carry both the charge and spin quantum numbers. We show that such quasiparticles arise as the dopant particles in the t-J model relevant for describing the SC phase. In particular, we formulate the RVB theory of the SC phase of the t-J model directly in terms of the dopant particles and apply it to describe the SC in the cobaltates.

Some earlier attempts have also been made to apply supersymmetry to study many–fermion interacting Hamiltonians as well as the t–J and related models. A linearization scheme for the general Hamiltonian of an interacting fermion system has been proposed in Ref. 14. A hierarchy of spectrum–generating algebras and superalgebras including su(2|1) results from such a new mean–field treatment. A supersymmetric representation of the Hubbard operator which unifies the slave–boson and slave–fermion representation into a single U(1|1) gauge theory has been developed in Ref. 15. Such a representation makes unnecessary the choice between a bosonic and fermionic spin and is most suitable to describe the coexistence of strong magnetic correlations within a paramagnetic phase. Besides, it has been demonstrated[16] that thus defined supersymmeric Hubbard operators prove to be very efficient in treating the physics of the infinite U Hubbard model.

III. SU(2|1) COHERENT STATES AND PATH INTEGRAL

The normalized su(2|1) coherent state (CS) associated with the 3D fundamental representation takes the form

$$|z,\xi\rangle = (1 + \bar{z}z + \bar{\xi}\xi)^{-1/2} \exp\left(zX^{\downarrow\uparrow} + \xi X^{0\uparrow}\right)|\uparrow\rangle, \quad (3)$$

where z is a complex number, and ξ is a complex Grassmann parameter. The set (z,ξ) can be thought of as local coordinates of a given point on $CP^{1|1}$. This supermanifold appears as a $N = 1$ superextension of a complex projective plane, or ordinary two–sphere, $CP^1 = S^2$, to accommodate one extra complex Grassmann parameter.[17] At $\xi = 0$, the su(2|1) CS reduces to the ordinary su(2) CS, $|z,\xi = 0\rangle \equiv |z\rangle$ parametrized by a complex coordinate $z \in CP^1$. Note that the classical phase space of the Hubbard operators, $CP^{1|1}$, appears as a $N = 1$ superextension of the CS manifold for the su(2) spins.

As is well known the key point in constructing the coherent–state path–integral representation of a partition function is the resolution of unity or, equivalently, the completeness relation for the coherent states. In terms of the normalized set of states (3) it takes the form

$$\int d\mu_{SU(2|1)} |z\xi\rangle\langle z\xi| = I,$$

where

$$d\mu_{SU(2|1)} = \frac{d\bar{z}dz}{2\pi i} \frac{d\bar{\xi}d\xi}{1 + |z|^2 + \bar{\xi}\xi}$$

stands for the SU(2|1) invariant measure on the coherent-state manifold, $CP^{1|1}=SU(2|1)/U(1|1)$, and I is the identity operator in the projected Hilbert space. Explicitly, we have

$$\int d\mu|z\xi\rangle\langle z\xi| = \int \frac{d\bar{z}dzd\bar{\xi}d\xi}{2\pi i(1 + |z|^2 + \bar{\xi}\xi)} |z\xi\rangle\langle z\xi|$$

$$= \int \frac{d\bar{z}dzd\bar{\xi}d\xi}{2\pi i(1 + |z|^2 + \bar{\xi}\xi)} \frac{1}{(1 + |z|^2 + \bar{\xi}\xi)}$$

$$\times \left(|\uparrow\rangle\langle\uparrow| + |z|^2|\downarrow\rangle\langle\downarrow| + \xi\bar{\xi}|0\rangle\langle 0|\right)$$

$$= |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |0\rangle\langle 0| \equiv I.$$

In the basis $|z,\xi\rangle = \prod_j |z_j,\xi_j\rangle$, the t–J partition function takes the form of the su(2|1) CS phase-space path integral,

$$Z_{t-J} = tr\ \exp(-\beta H_{t-J}) = \int_{CP^{1|1}} D\mu_{SU(2|1)}(z,\xi)\, e^{S_{t-J}}, \quad (4)$$

where

$$D\mu_{SU(2|1)}(z,\xi) = \prod_{j,t} \frac{d\bar{z}_j(t)dz_j(t)}{2\pi i} \frac{d\bar{\xi}_j(t)d\xi_j(t)}{1 + |z_j|^2 + \bar{\xi}_j\xi_j}$$

stands for the SU(2|1) invariant measure with the boundary conditions, $z_j(0) = z_j(\beta)$, $\xi_j(0) = -\xi_j(\beta)$. The t-J effective action on $CP^{1|1}$ now reads $S_{t-J} = -\int_0^\beta \langle z,\xi|d/dt + H_{t-J}|z,\xi\rangle dt$, which gives

$$S_{t-J} = \frac{1}{2}\sum_j \int_0^\beta \frac{\dot{\bar{z}}_j z_j - \bar{z}_j\dot{z}_j + \dot{\bar{\xi}}_j\xi_j - \bar{\xi}_j\dot{\xi}_j}{1 + |z_j|^2 + \bar{\xi}_j\xi_j}dt$$

$$- \int_0^\beta H_{t-J}^{cl}dt. \quad (5)$$

The first part of the action (5) is a purely kinematical term that reflects the geometry of the underlying phase space while the classical image of the Hamiltonian (2) becomes an average value of H_{t-J} over the su(2|1) coherent states,

$$H_{t-J}^{cl} = \langle z,\xi|H_{t-J}|z,\xi\rangle$$

$$= -t\sum_{ij} \frac{\xi_i\bar{\xi}_j(1 + z_j\bar{z}_i) + h.c.}{(1 + |z_i|^2 + \bar{\xi}_i\xi_i)(1 + |z_j|^2 + \bar{\xi}_j\xi_j)}$$

$$+ J\sum_{ij} \frac{-|z_i|^2 - |z_j|^2 + z_iz_j + \bar{z}_i\bar{z}_j}{(1 + |z_i|^2 + \bar{\xi}_i\xi_i)(1 + |z_j|^2 + \bar{\xi}_j\xi_j)}.$$

$$(6)$$

The fact that the electron system with the NDO constraint lives on the compact manifold, supersphere $CP^{1|1}$

can be explained as follows. Let us for a moment suppose that the so-called slave-fermion representation for the electron operators is used, i.e.,

$$c_{i\sigma} = f_i a_{i\sigma}^\dagger, \qquad (7)$$

where f_i is a on-site spinless fermionic operator, whereas $a_{i\sigma}$ is the spinful boson. The NDO constraint now reads $\sum_\sigma a_{i\sigma}^+ a_{i\sigma} + f_i^+ f_i = 1$. Within the slave-fermion path integral representation

$$Z_{t-J} = \int D\mu_{flat}\, e^{S_{t-J}(\overline{a}_\sigma, a_\sigma, f)}, \qquad (8)$$

with the integration measure $D\mu_{flat} = \prod_i D\overline{a}_{i\uparrow} Da_{i\uparrow} D\overline{a}_{i\downarrow} Da_{i\downarrow} D\overline{f}_i Df_i$, this constraint transforms into

$$\sum_\sigma \overline{a}_{i\sigma} a_{i\sigma} + \overline{f}_i f_i = 1, \qquad (9)$$

with $a_{i\sigma}$ and f_i standing now for complex numbers and complex Grassmann parameters, respectively. Equation (9) is exactly that for the supersphere $CP^{1|1}$ embedded into a flat superspase. Any mean-field treatment of (8) should respect this constraint, which, however, poses a severe technical problem. If one however resolves this equation explicitly by making the identifications

$$a_{i\uparrow} = \frac{e^{i\phi_i}}{\sqrt{1 + \overline{z}_i z_i + \overline{\xi}_i \xi_i}}, \; a_{i\downarrow} = \frac{z_i e^{i\phi_i}}{\sqrt{1 + \overline{z}_i z_i + \overline{\xi}_i \xi_i}},$$
$$f_i = \frac{\xi_i e^{i\phi_i}}{\sqrt{1 + \overline{z}_i z_i + \overline{\xi}_i \xi_i}}, \qquad (10)$$

one can further treat the variables z_i, ξ_i as if they were indeed free of any constraints.

Note that the electron operator (7) is invariant under a local gauge transformation,

$$a_{i\sigma} \to a_{i\sigma} e^{i\theta_i}, \quad f_i \to f_i e^{i\theta_i},$$

or equivalently, under the change $\phi_i \to \phi_i + \theta_i$. This gauge symmetry is a consequence of the redundancy of parameterizing the electron operator in terms of the auxiliary boson/fermion fields. In contrast, the $su(2|1)$ projected coordinates

$$z_i = a_{i\downarrow}/a_{i\uparrow}, \quad \xi_i = f_i/a_{i\uparrow}$$

are seen to be manifestly gauge invariant. The domain of the flat measure in (8) that involves the spin up bosonic fields can be rewritten at every lattice site as $D\overline{a}_{i\uparrow} Da_{i\uparrow} = D|a_{i\uparrow}|^2 D\phi_i$. The $|a_{i\uparrow}|^2$ field can easily be integrated out from eq.(8) because of the constraint (9). Since the t-J action is U(1) gauge invariant and hence independent of ϕ_i, the integration over ϕ_i results in merely some numerical factor that can be taken care of by a proper normalization of the partition function. For the remaining integration we have (the site dependence for the moment being suppressed),

$$Da_\downarrow D\overline{a}_\downarrow Df D\overline{f} = \mathrm{sdet}\|\frac{\partial(a_\downarrow, \overline{a}_\downarrow, f, \overline{f})}{\partial(z, \overline{z}, \xi, \overline{\xi})}\|\, Dz D\overline{z} d\xi D\overline{\xi}.$$

The Jacobian of the change of the supercoordinates appears as a superdeterminant of the transformation matrix[18]

$$\mathrm{sdet}\|\frac{\partial(a_\downarrow, \overline{a}_\downarrow, f, \overline{f})}{\partial(z, \overline{z}, \xi, \overline{\xi})}\| = \mathrm{sdet}\begin{pmatrix} A & B \\ C & D \end{pmatrix}$$
$$:= \det(A - BD^{-1}C)\det D^{-1}.$$

Here

$$A = \begin{pmatrix} \frac{\partial a_\downarrow}{\partial z} & \frac{\partial a_\downarrow}{\partial \overline{z}} \\ \frac{\partial \overline{a}_\downarrow}{\partial z} & \frac{\partial \overline{a}_\downarrow}{\partial \overline{z}} \end{pmatrix}, \quad B = \begin{pmatrix} \frac{\partial a_\downarrow}{\partial \xi} & \frac{\partial a_\downarrow}{\partial \overline{\xi}} \\ \frac{\partial \overline{a}_\downarrow}{\partial \xi} & \frac{\partial \overline{a}_\downarrow}{\partial \overline{\xi}} \end{pmatrix},$$

$$C = \begin{pmatrix} \frac{\partial f}{\partial z} & \frac{\partial f}{\partial \overline{z}} \\ \frac{\partial \overline{f}}{\partial z} & \frac{\partial \overline{f}}{\partial \overline{z}} \end{pmatrix}, \quad D = \begin{pmatrix} \frac{\partial f}{\partial \xi} & \frac{\partial f}{\partial \overline{\xi}} \\ \frac{\partial \overline{f}}{\partial \xi} & \frac{\partial \overline{f}}{\partial \overline{\xi}} \end{pmatrix},$$

with the derivatives with respect to the Grassmann parameters ξ and $\overline{\xi}$ being understood to be the right ones.

Evaluating the superdeterminant

$$\mathrm{sdet}\|\frac{\partial(a_\downarrow, \overline{a}_\downarrow, f, \overline{f})}{\partial(z, \overline{z}, \xi, \overline{\xi})}\| = \frac{1}{1 + |z|^2 + \overline{\xi}\xi}$$

and substituting of (10) into (8) we are led to the su(2|1) path-integral representation of Z_{t-J} given by (4). Note that the U(1) gauge field ϕ_i drops out from representation (4). An attempt at decoupling the physical electron as a U(1) gauge invariant "dressed" holon and spinon has been made in Ref. 19.

Geometrically, the set (z, ξ) appears as local (inhomogeneous) coordinates of a point on the supersphere defined by equation (9). Representation (4)-(6) rigorously incorporates the local NDO constraint at the apparent expense of a more complicated compact phase space for the projected electron operators.

IV. SYMMETRY

At the supersymmetric point, $J = 2t$, the $t-J$ model Hamiltonian is known to exhibit a global SU(2|1) symmetry. Away from that point this symmetry reduces to SU(2)$\times$ U(1)$\subset$ SU(2|1). This symmetry group acts on a point $(z(t), \xi(t)) \in CP^{1|1}$ in a way that,

$$z(t) \to z_g(t) = \frac{uz(t) + v}{-\overline{v}z(t) + \overline{u}}, \quad g \in \mathrm{SU}(2) \times \mathrm{U}(1),$$

$$\xi(t) \to \xi_g(t) = \frac{e^{i\theta}\xi(t)}{-\overline{v}z(t) + \overline{u}}, \qquad (11)$$

where the group parameters are to be taken to be site independent:

$$\begin{pmatrix} u & v \\ -\overline{v} & \overline{u} \end{pmatrix} \in SU(2), \quad e^{i\theta} \in U(1). \tag{12}$$

It can easily be checked that both the SU(2|1) measure and the effective action (5) are invariant under the group transformations (11), so that the representation of the partition function (4) remains intact. Notice that (11) appears as a covariant reparametrization of $CP^{1|1}$. However, one can in principle employ any other reparametrization, not necessarily of the form of the SU(2|1) action on $CP^{1|1}$. We are interested in the one that decouples the SU(2|1) measure factor into the SU(2) spin and the U(1) spinless fermion measures,

$$\begin{aligned} D\mu_{SU(2)}(\overline{z}, z) &= \prod_{j,t} \frac{d\overline{z}_j(t) dz_j(t)}{2\pi i (1 + |z_j(t)|^2)^2}, \\ D\mu_{U(1)}(\overline{\xi}, \xi) &= \prod_{j,t} d\overline{\xi}_j(t) d\xi_j(t), \end{aligned}$$

respectively.

Such a reparametrization can be taken to be

$$z \to z, \ \xi \to \xi\sqrt{1 + |z|^2}. \tag{13}$$

Up to an inessential factor which redefines a chemical potential, we get

$$D\mu_{su(2|1)} \to D\mu_{su(2)}(\overline{z}, z) \times D\mu_{u(1)}(\overline{\xi}, \xi), \tag{14}$$

and the effective action becomes

$$S_{t-J} \to S_{t-J} = \frac{1}{2} \sum_i \int_0^\beta \frac{\overline{\dot{z}}_i z_i - \overline{z}_i \dot{z}_i}{1 + \overline{z}_i z_i} (1 - \overline{\xi}_i \xi_i) dt$$
$$+ \frac{1}{2} \sum_i \int_0^\beta (\overline{\dot{\xi}}_i \xi_i - \overline{\xi}_i \dot{\xi}_i) dt - \int_0^\beta \widetilde{H}_{t-J}^{cl}(t) dt, \tag{15}$$

with

$$\widetilde{H}_{t-J}^{cl} = -t \sum_{ij} (\xi_i \overline{\xi}_j \langle z_i | z_j \rangle + h.c.)$$
$$+ \frac{J}{2} \sum_{ij} \left(|\langle z_i | z_j \rangle|^2 - 1 \right) \left(1 - \overline{\xi}_i \xi_i \right) \left(1 - \overline{\xi}_j \xi_j \right). \tag{16}$$

Here $\langle z_i | z_j \rangle$ stands for an inner product of the su(2) coherent states,

$$\langle z_i | z_j \rangle = \frac{1 + \overline{z}_i z_j}{\sqrt{(1 + |z_j|^2)(1 + |z_i|^2)}}.$$

From eqs. (11) one can infer the transformation properties of the new $CP^{1|1}$ coordinates (13) under a global SU(2)×U(1) action:

$$\begin{aligned} z(t) \to z_g(t) &= \frac{uz(t) + v}{-\overline{v}z(t) + \overline{u}}, \\ \xi(t) \to \xi_g(t) &= e^{i\phi_g + i\theta} \xi(t), \end{aligned} \tag{17}$$

where

$$i\phi_g = \ln\sqrt{\frac{-v\overline{z} + u}{-\overline{v}z + \overline{u}}}.$$

Note also that $|z\rangle \to |z\rangle_g = e^{-i\phi_g}|z_g\rangle$. It can be straightforwardly checked that both the measure and the t-J action (15) remain invariant, under such an action of SU(2)×U(1).

The following remarks are needed at this stage. First, in spite of the fact that the function $i\phi_g$ bears a site-dependence through the z_i fields, the transformation (17) is a global one: the group parameters (u, v) are site-independent. Second, although the measure factor gets decomposed into the su(2) spin and spinless fermion pieces, the underlying phase space is not reduced into a direct product of the classical spin and a flat fermionic phase spaces. The function ϕ_g that enters the transformation law for the fermions also depends on the spinon coordinates, $z_i(t)$. Besides, the symplectic one-form (kinetic term) in the effective action (15) is not a simple sum of purely fermionic and spin contributions. This means physically that, in general, the corresponding field excitations are not independent of each other. In the other words, the spin-charge separation does not merely reduce to a simple (z, ξ) representation, and should, in fact, be described by nonlocal 'string' excitations to be constructed out of the basic (z, ξ) fields.

V. EFFECTIVE ACTION

The spinon amplitudes $z_i(t)$ and the spinless fermion parameters, $\xi_i(t)$, are in fact related to each other by the SU(2) transformation laws (17). From this it follows that we can construct classical images[20] for the operators that describe doped holes. In this respect we make the following ansatz:

$$\begin{aligned} \Psi_\downarrow &= \frac{-\xi}{\sqrt{1 + |z|^2}}, \ \overline{\Psi}_\downarrow = \frac{-\overline{\xi}}{\sqrt{1 + |z|^2}}, \\ \Psi_\uparrow &= \frac{\overline{z}\xi}{\sqrt{1 + |z|^2}}, \ \overline{\Psi}_\uparrow = \frac{z\overline{\xi}}{\sqrt{1 + |z|^2}}. \end{aligned} \tag{18}$$

It then follows that $\overline{\Psi}_\uparrow \Psi_\uparrow + \overline{\Psi}_\downarrow \Psi_\downarrow = \overline{\xi}\xi = \widehat{\delta}^{cl}$, where $\widehat{\delta}^{cl}$ stands for a classical image of the hole–number operator $\widehat{\delta} = 1 - \widehat{n}_e = 1 - \sum_\sigma X^{\sigma\sigma}$. Therefore the resulting fermionic amplitudes describe the propagation of doped holes restricted to the NDO constraint. In view of the group transformations SU(2)×U(1) for $z(t)$ and $\xi(t)$ the Ψ_σ amplitudes transform in a *linear* spinor representation of SU(2) as true fermionic amplitudes. Namely,

$$\begin{pmatrix} \Psi_\uparrow \\ \Psi_\downarrow \end{pmatrix} \to \begin{pmatrix} \overline{u} & -\overline{v} \\ v & u \end{pmatrix} \begin{pmatrix} \Psi_\uparrow \\ \Psi_\downarrow \end{pmatrix} \tag{19}$$

In terms of the Ψ_σ and z amplitudes we get the corresponding *exact* representation of the $t-J$ partition func-

tion,

$$Z_{t-J} = \int D\mu_{SU(2)}(\overline{z}, z)D\mu_{U(1)}(\overline{\Psi}, \Psi) \exp S$$
$$\times \prod_i \delta\left(\frac{\Psi_{\uparrow i} + \overline{z}_i \Psi_{\downarrow i}}{\sqrt{1 + |z_i|^2}}\right) \delta\left(\frac{\overline{\Psi}_{\uparrow i} + z_i \overline{\Psi}_{\downarrow i}}{\sqrt{1 + |z_i|^2}}\right), (20)$$

where

$$S = S_{kin} - \int_0^\beta \tilde{H}_{t-J}^{cl}(t)dt. \qquad (21)$$

The SU(2) invariant product of the δ - functions ensures the preservation of the correct number of degrees of freedom. The square roots in the δ- function arguments come from the evaluation of the Jacobian. In this new dopant carrier representation the kinetic term,

$$S_{kin} = \frac{1}{2}\sum_{\sigma i} \int_0^\beta \left(\overline{\dot{\Psi}}_{\sigma i}\Psi_{\sigma i} - \overline{\Psi}_{\sigma i}\dot{\Psi}_{\sigma i}\right) dt$$
$$+ \frac{1}{2}\sum_i \int_0^\beta \frac{\overline{\dot{z}}_i z_i - \overline{z}_i \dot{z}_i}{1 + \overline{z}_i z_i} dt, \qquad (22)$$

is nicely decoupled into purely fermionic and spinon parts. It is clear that the fermionic symplectic one–form (the first term in (22)) determines a standard fermionic symplectic structure $\sum_\sigma d\overline{\Psi}_\sigma \wedge d\Psi_\sigma$ which in turn determines the standard Poisson brackets relations $\{\overline{\Psi}_\sigma, \Psi_{\sigma'}\}_{PB} = \delta_{\sigma,\sigma'}, \{\Psi_\sigma, \Psi_{\sigma'}\}_{PB} = 0$. As a result the corresponding operators Ψ_σ^+, $\Psi_{\sigma'}$ describe indeed well-defined fermionic excitations - in our case, doped holes.

As a result, using the new fermion fields, the Hamiltonian that corresponds to $\tilde{H}_{t-J}^{cl}$ takes the form

$$H_{t-J} = t\sum_{ij\sigma} \Psi_{i\sigma}^+ \Psi_{j\sigma} + h.c. + J\sum_{ij} \left[(\overrightarrow{S}_i \overrightarrow{S}_j - \frac{1}{4})\right.$$
$$\left. + (\overrightarrow{S}_i \overrightarrow{M}_j + \overrightarrow{S}_j \overrightarrow{M}_i) + (\overrightarrow{M}_i \overrightarrow{M}_j - \frac{1}{4}\hat{\delta}_i\hat{\delta}_j)\right], (23)$$

where we have dropped the tilda sign. The components of the operator of spinon magnetic moment $\overrightarrow{S}$ are the su(2) generators in the $s = \frac{1}{2}$ representation . Their classical images are the components of $\overrightarrow{S}^{cl} = \langle z|\overrightarrow{S}|z\rangle$ with $(\overrightarrow{S}^2)_{cl} = \frac{3}{4}$. The hole spin operator $\overline{M} = \frac{1}{2}\sum_\sigma \Psi_\sigma^+ \overrightarrow{\tau}_{\sigma\sigma'}\Psi_\sigma$, $\overline{M}^2 = \frac{3}{4}\hat{\delta}\left(2 - \hat{\delta}\right), \hat{\delta} = \Psi_\uparrow^+ \Psi_\uparrow + \Psi_\downarrow^+ \Psi_\downarrow$, transforms under (17), as a SU(2) vector while the total hamiltonian (23) is a SU(2) scalar. It can also be checked that the electron spin moment is a linear combination of the above two operators: $\overrightarrow{Q} = \overrightarrow{S} + \overline{M}$. If we integrate out the fields $\Psi_{\uparrow i}, \overline{\Psi}_{\uparrow i}$ in Eq. (20), with the help of the $\delta-$ functions, we will return to our initial representation as given in Eq. (15).

Different parts of the Hamiltonian (23) can be associated with the different phases of the t-J model. For a half-filled band, Eq. (23) reduces to the Heisenberg antiferromagnet (AF), $H_{t-J}^{AF} = J\sum_{ij}(\overrightarrow{S}_i \overrightarrow{S}_j - \frac{1}{4})$. Away

from half-filling in the lightly doped regime, where δ is small enough, so that one can ignore a direct hole-hole interaction, the Hamiltonian

$$H_{t-J}^{AF-PG} = t\sum_{ij\sigma} \Psi_{i\sigma}^+ \Psi_{j\sigma} + h.c. + J\sum_{ij} \left[(\overrightarrow{S}_i \overrightarrow{S}_j - \frac{1}{4})\right.$$
$$\left. + (\overrightarrow{S}_i \overrightarrow{M}_j + \overrightarrow{S}_j \overrightarrow{M}_i)\right], \qquad (24)$$

is able to describe the AF - pseudogap (PG) transition on a square lattice. Accordingly, at higher doping, the Hamiltonian

$$H_{t-J}^{PG-SC} = t\sum_{ij\sigma} \Psi_{i\sigma}^+ \Psi_{j\sigma} + h.c. + J\sum_{ij} \left[\overrightarrow{S}_i \overrightarrow{M}_j\right.$$
$$\left. + \overrightarrow{S}_j \overrightarrow{M}_i + (\overrightarrow{M}_i \overrightarrow{M}_j - \frac{1}{4}\hat{\delta}_i\hat{\delta}_j)\right], \qquad (25)$$

is appropriate for the pseudogap - superconductor boundary region of the t-J phase diagram.

The PG phase itself can be described within our approach by a simple SU(2) invariant spinon-fermion interaction,

$$H_{t-J}^{PG} = t\sum_{ij\sigma} \Psi_{i\sigma}^+ \Psi_{j\sigma} + h.c.$$
$$+ J\sum_{ij} \left[\overrightarrow{S}_i \overrightarrow{M}_j + \overrightarrow{S}_j \overrightarrow{M}_i\right]. \qquad (26)$$

To see this, one can recast the Hamiltonian (26) into the form of the phenomenological boson - fermion model (BFM) which is known to capture the main observable characteristic of the PG phenomenon, namely the reduction of the fermionic density of states at the Fermi level[21]. Using the Holstein-Primakoff (HP) representation of the spin operators on the bipartite lattice $L = A \bigoplus B$,

$$S_i^z = 1/2 - b_i^\dagger b_i, \quad S_i^+ = -b_i, \quad S_i^- = -b_i^\dagger, \quad i \in A,$$

$$S_i^z = 1/2 - b_i^\dagger b_i, \quad S_i^+ = b_i, \quad S_i^- = b_i^\dagger, \quad i \in B,$$

where $[b, b^\dagger] = 1$, and performing the following unitary transformation of the fermionic operators

$$\Psi_{\uparrow i} \to \Psi_{\uparrow i}^\dagger, i \in A, \quad \Psi_{\uparrow i} \to -\Psi_{\uparrow i}^\dagger, i \in B,$$

one is led to the BFM - type Hamiltonian

$$H_{t-J}^{PG} \to H^{BFM} = t\sum_{ij} \Psi_{i\sigma}^+ \Psi_{j\sigma} + h.c. - J\sum_i \Psi_{i\sigma}^\dagger \Psi_{i\sigma}$$
$$- 2J\sum_i b_i^\dagger b_i + J\sum_{ij} (\Psi_{\uparrow j}\Psi_{\downarrow j}b_i^\dagger + h.c)$$
$$+ \lambda\sum_i (2b_i^\dagger b_i + \Psi_{i\sigma}^\dagger \Psi_{i\sigma} - 2), \qquad (27)$$

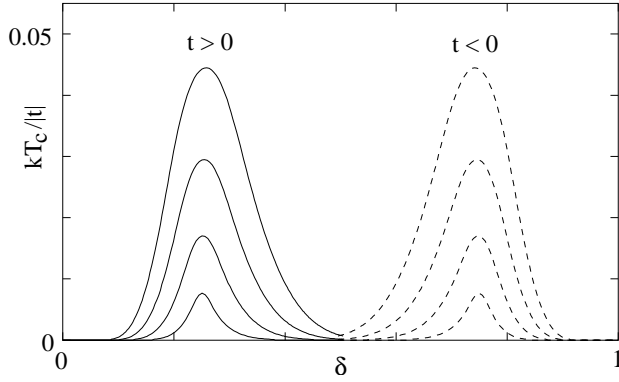FIG. 1: $T_c(\delta)$ for negative and positive t. The curves from the bottom to the top correspond to $J/|t|$ =0.6, 0.8, 1, 1.2.
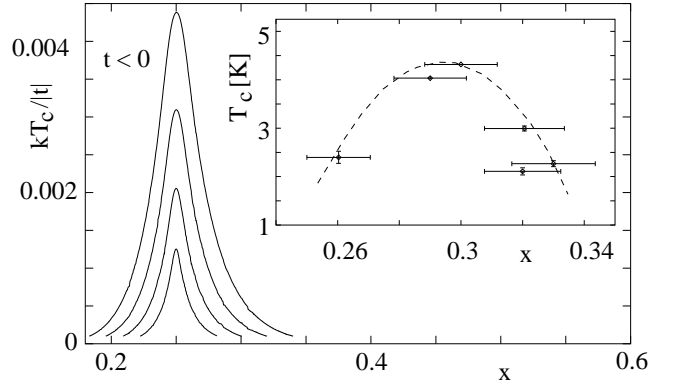

FIG. 2: T_c as a function of doping for $t < 0$. The curves from the bottom to the top correspond to $J/|t|$ =0.35, 0.4, 0.45, 0.5. For comparison, the insert shows experimental data for $Na_x CoO_2 \cdot yH_2O$ taken from Ref.[2].

with the implied summation over σ. The Lagrange multiplier λ has been introduced to enforce the constraint which assures the vanishing of the total electron spin projection, $< 2Q^z >= 0$. Notice that due to the global U(1) invariance the conditions $< Q^{\pm} >= 0$ are automatically satisfied. While both the conventional BFM and H_{t-J}^{PG} Hamiltonians possess the same global symmetry, namely SU(2)$\times$ U(1), with the $SU(2)$ group describing of the rotation of the spinor fields, the origin of the U(1) symmetry is different in the two cases. In the standard BFM, the global U(1) symmetry corresponds to the conservation of the total charge of bosons and fermions. Here the U(1) symmetry group appears just as a subgroup of the explicitly broken (by the HP representation) total spin rotation group, generated by the operators $\vec{Q}s$. Therefore, despite the formal similarity between those two effective models, the physical contents of the standard BFM and the representation (27) are indeed different from each other .

Note, finally, that our discussed hierarchy of effective t-J Hamiltonians is basically qualitative in the sense that the constraint imposed by the δ-functions might change their detailed forms. While this constraint does not seem to be of the crucial importance at very low density of dopant carriers, it definitely becomes more important as δ increases, and this may in turn substantially affect the final form of the effective interactions. However, since the global SU(2) invariance of the t-J Hamiltonian (23) is not affected by the constraint, it is plausible to suggest that those changes will at most, at the mean-field level, result merely in a renormaization of the Hamiltonian parameters similar to what happens to the t and J parameters in the mean-field Plain Vanilla theory[22]. We intend to address these problems in more detail in a separate publication.

VI. SC PHASE

The RVB mean field treatment of the SC phase of the Hamiltonian (23) is now based on the following assumptions:

i) the global SU(2)$\times$U(1) symmetry is spontaneously broken by a local order parameter down to SU(2). The SU(2) symmetry is the exact symmetry of the SC phase; ii) the dynamics of the SC phase is governed by the BCS–type dynamics of the valence bond *hole* SU(2) singlet pairs and is determined by the linearized hole–hole interaction $J \sum_{ij} \left(\vec{M}_i \vec{M}_j - \frac{1}{4} \widehat{\delta}_i \widehat{\delta}_j \right)$ as well as by the hopping term. The hole spin singlets interact with the quasi-classical spinon background $J \sum_{ij} \left(\vec{S}_i \vec{S}_j - \frac{1}{4} \right)$ via the induced moment-moment interaction $J \sum_{ij} \vec{S}_i \vec{M}_j$. This can be treated within the MF approximation as well. However, for the cobaltates we ignore, at first, quantum fluctuation effects of the spinon field in comparison with the ones originated by the Ψ–field.[23] In contrast, for the cuprates the $\langle \vec{S}_i \vec{M}_j \rangle$ correlation functions seem to be of crucial importance and should therefore be treated beyond a MF approximation. This is confirmed by the observation of antiferromagnetic ordering associated with the superconducting vortex cores;[24] iii) the constrained RVB hole-singlet annihilation operator takes the form $B_{ij} = \Psi_{i\uparrow} \Psi_{j\downarrow} - \Psi_{i\downarrow} \Psi_{j\uparrow}$, $B_{ii} = 0$. In the SC phase the $U(1)$ global symmetry $\Psi_{j\sigma} \rightarrow e^{i\theta} \Psi_{j\sigma}$ is spontaneously broken by the local SU(2) invariant order parameter $\Delta_{ij} = \langle B_{ij} \rangle$.

The t–J Hamiltonian function in Eq.(21) now reduces to

$$H_{t-J}^{SC} = t \sum_{ij\sigma} \bar{\Psi}_{i\sigma} \Psi_{j\sigma} + h.c. + \frac{JNZ|\Delta|^2}{4} - N_e \mu$$

$$+ \frac{J}{2} \sum_{ij} \left(\Psi_{i\uparrow} \Psi_{j\downarrow} - \Psi_{i\downarrow} \Psi_{j\uparrow} \right) \overline{\Delta}_{ij} + h.c. \quad (28)$$

where the chemical potential μ has been introduced to control the number of electrons, $\widehat{N}_e = N - \sum_{\sigma i} \Psi_{i\sigma}^+ \Psi_{i\sigma}$. This Hamiltonian continues to be invariant under the $SU(2)$ action induced by (19).

Despite its similar appearance with the standard MF RVB result[9], eq.(28) has a different content. The most important difference is related to the presence of constraints imposed by the δ–functions in Eq. (20). However, even if these functions are neglected, the Hamiltonian (28) deals directly with the dopant–particle operators $\Psi_{i\sigma}$'s rather than with the electron operators $c_{i\sigma}$'s. In terms of $\Psi_{i\sigma}$'s, $\widehat{N}_e$ has a different representation, and a different equation for the chemical potential follows from that. As a consequence, within our approach a nonzero Δ directly implies superconductivity in contrast to the original BZA approach, where at half-filling Δ^{BZA} is nonzero, but the state is insulating.

Due to the fact that we are directly dealing with the dopant particles T_c vanishes for $\delta = 0$. Moreover, the average of the kinetic term in $H_{t-J}^{SC} \sim t\delta$. The increase of δ reflects itself in the gain of kinetic energy which will eventually be of the order of J. When this occurs the singlet pairs tend to break up and the SC phase disappears. Strictly speaking T_c is non-zero for any non-vanishing δ (see Fig. 1). This is an artifact of the applied MF approximation since it neglects a possible onset of magnetic ordering.[7] In the standard RVB decoupling scheme the J–term vanishes above the RVB transition temperature. Therefore, the resulting phase diagram for the square lattice usually does not include the AF phase for the half-filled case. In the present approach the J-term is expressed as a sum of spinon, dopant and spinon-dopant terms (see Eq. (23)). The introduced above RVB state naturally disappears at half-filling and the Hamiltonian (23) is reduced to the Heisenberg one. Therefore, for $\delta = 0$, the system becomes insulating and the ground state energy can only be lowered by the onset of the magnetic phase. In particular, for the square lattice one expects the onset of the long range order antiferromagnetic order. In order to determine the actual boundary of the magnetic phase, one should consider it together with the RVB phase, since these phases compete with each other.

A few remarks are in order. Since the RVB singlets are doped hole–hole pairs the present MF favors larger hole doping in contrast to the BZA scheme. Thus the present approach must be more reliable for the t–J interaction on a triangular lattice.

It can be shown (see Appendix) that the equations for the order parameter and the chemical potential that follow from the partition function representation (20) with the MF BCS Hamiltonian (28) are invariant under the change $t \to -t$, $\delta \to 1 - \delta$, $\mu \to -\mu$. Thus the NDO constraint imposes within the MF BCS approximation a symmetry restriction on a possible structure of the phase diagram. Namely, the phase diagrams $T_c(\delta)$ at $t > 0$ and $t < 0$ must be located symmetrically with respect to the point $\delta = \frac{1}{2}$. Any renormalization of the type $t \to \delta t$, frequently used in order to implement the constraint of no double occupancy in the MF BCS scheme, evidently spoils this symmetry.

Finally, Eq. (28) corresponds to hole doping. However, as already mentioned earlier on, the CoO_2's are more likely electron doped compounds. In order to deal with this case, within the representation (28), we make a canonical transformation $\Psi_\sigma \to \Psi_{-\sigma}^+$ and keep the NDO constraint as before. In its new form the operator Ψ_σ^+ creates a dopant electron. The phase diagram $T_c \times \delta$ which follows from our new "dual" RVB scheme is shown in Fig. 1, for hole doping. If we replace $\delta \to x, t \to -t$ we reproduce the main figure for the electron doping case. Our results for this case are shown in Fig. 2. In the insert of this figure we reproduce the experimental data from Schaak *et al.*[2] for comparison.

This phase diagram is evaluated directly from Eq. (28) considering a triangular lattice of CoO_2's. The $d + id$ symmetry of the MF OP predicted earlier in Refs. 4,5 and 25 is employed throughout the calculations. Other symmetries can be tested if necessary using the same scheme. The representation (20) with the Hamiltonian function given by Eq. (28) incorporates the NDO constraint rigorously and tells us that at most one spinful fermion can live on a given lattice site. Technically, the problem reduces to a computation of the fermionic determinant in the presence of the constraints imposed by the δ-functions.

The fermionic determinant arises upon integrating a bilinear form in the exponential over the complex spinors $\Sigma_{\overrightarrow{k},\varpi_n} \equiv \left(\overline{\Psi}_{\uparrow \overrightarrow{k},\varpi_n}, \Psi_{\downarrow -\overrightarrow{k},-\varpi_n} \right)$. Here $\varpi_n = \frac{\pi}{\beta}(2n+1)$ stands for the Matsubara fermionic frequency and vector $\overrightarrow{k} \in BZ$. Had there been no δ-functions in (20) the amplitudes $\Sigma_{\overrightarrow{k},\varpi_n > 0}$ and $\Sigma_{\overrightarrow{k},\varpi_n < 0}$ would have been completely independent and contributed equally to the partition function. In the presence of the δ-functions, however, those amplitudes are no longer independent.

The δ–functions result in some interference between these amplitudes reducing the total contribution to the partition function. In order to estimate this reduction at the mean–field level we use the following trick. We multiply the piece of the free energy that comes from the evaluation of the determinant at the absence of the constraints by a coefficient $\kappa < 1$. Then, requiring that resulting equations for the order parameter and the chemical potential be invariant under the change $t \to -t$, $\delta \to 1 - \delta$, and $\mu \to -\mu$ gives $\kappa = 1/2$.

Although this approximation cannot be justified rigorously, it goes beyond the one based on the renormalization of the hopping term in the form, $t \to \delta t$, which is frequently used to partly take into account the restriction of no double occupancy. In particular, our approximation does not spoil the already mentioned symmetry of the MF phase diagram under the changes $t \to -t$, $\delta \to 1 - \delta$ dictated by the NDO constraint (see Fig. 1 and the Appendix). However, a more detailed analysis must take into account a rigorous treatment of the delta–function contribution.

Our results for $Na_x CoO_2 \cdot yH_2O$ are very suggestive since the experimentally observed dome structure of the phase diagram is reproduced by theoretical calculations within a RVB framework. The obtained widths for the

dome are also of the same magnitude as given by experiments,[2,3] although our doping values are somewhat shifted toward the origin. However, recent experimental results[26] indicate that the actual hole concentration in the cobalt planes may differ from that estimated solely on the basis of the Na content and the optimal doping can be shifted from the value reported in Ref.2. The precise value of J for this compound is still unknown. However for $t = -0.1$eV and $J/|t|$ ranging from 0.35 to 0.5 as depicted in Figure 2, max T_c varies roughly from $1K$ to $4K$. Our mean field results are, therefore, in good agreement with the existing experimental data.

The obtained phase diagram is asymmetric with respect to the change $t \to -t$ (electron and hole doping). The $t \to -t$ asymmetry has also been obtained in Ref. 6 within a MF slave–boson Hamiltonian. In both MF approaches this asymmetry is an obvious consequence of the free–particle dispersion relation on the triangular lattice. In our case, this asymmetry concerns only the different values of the optimal doping in electron– and hole–doped systems. In Ref. 6, it is associated predominantly with the different width of the SC region in the $T_c \times \delta$ phase diagram for different doping regimes. Additionally, we have obtained much larger value of the optimal doping than that reported in Ref. 6. Note, that the maximal value of T_c obtained in Ref. 6 for the case of electron doping is close to that obtained for the hole doping.

According to our knowledge, there is however no experimental verification concerning the explicit form of this asymmetry in contrast to the electron–hole asymmetry observed in cuprate superconductors. The t–J Hamiltonians (1) on a square lattice with double/zero occupancy for hole/electron doping are unitary equivalent. Accordingly, on a square lattice there is no asymmetry with respect to the change $t \to -t$. In fact, the doping asymmetry in the high–T_c cuprates has quite a different origin. A possible resolution of this puzzle has recently been provided within a two–species t-J model in Ref. 27.

The doping dependence of the superfluid stiffness D_s is an important ingredient of the standard RVB theory as discussed in Ref. 22. In particular, small values of D_s for $\delta \to 0$ determine the superconducting transition temperature. This quantity can be obtained with the help of the linear response theory from the relation between the current and the transverse gauge field. The response kernel consists of paramagnetic and diamagnetic parts. In the superconducting state (or more precisely for $\Delta \neq 0$) the paramagnetic contribution vanishes for $T \to 0$.[28] It has been shown that the diamagnetic part imposes also the upper bound on D_s.[29] In the case of the hypercubic lattice with the nearest–neighbor hopping, D_s/π is bounded by the absolute value of the kinetic energy on a bond, whereas for a more general dispersion relation $\varepsilon(\vec{k})$ the kinetic energy should be replaced by[29]

$$K(T) = \frac{1}{N} \sum_{\vec{k} \in BZ} n(\vec{k}) \mathrm{Tr} \left[m^{-1}(\vec{k}) \right],$$
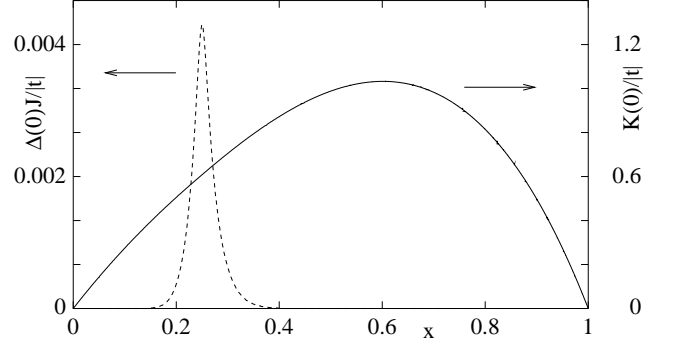

FIG. 3: Doping dependence of $K(T)$ and $\Delta(T)$ obtained for the triangular lattice with $J/|t| =0.5$ and $T \to 0$.

where $m_{ab}^{-1}(k) = \partial^2 \varepsilon(\vec{k})/\partial k_a \partial k_b$. In order to estimate the magnitude of the superfluid stiffness in our approach, we have calculated $T = 0$ limit of this quantity. Fig 3. shows the doping dependences of $K(0)$ and $\Delta(0)$. In the standard RVB approach the NDO constraint $t \to \delta t$ renormalizes the superfluid stiffness since it modifies the kinetic energy. Consequently, close to half–filling D_s vanishes despite the finite value of Δ.[22] In this regime $T_c \sim D_s \sim \delta$. In our approach the superfluid stiffness vanishes for the half–filling as well. Since the kinetic energy term in Eq. (23) contains only the dopant particles the vanishing of the superfluid stiffness for $\delta \to 0$ is an intrinsic feature of our approach and occurs independently of the applied approximations.

We end this section discussing briefly how one can control the BCS mean–field decoupling (28) within the su(2|1) supersymmetric representation of the Hubbard operators. This can be done by means of a large–N expansion based on a generalization of the SU(2) globally invariant t–J Hamiltonian (2) in terms of the symplectic group Sp(2N) of 2N× 2N unitary matrices (note that Sp(2)$\cong$ SU(2))[15,30,31]:

$$H_{t-J}^{SU(2)} \to H_{t-J}^{Sp(2N)} = -t \sum_{ij} X_i^{\sigma 0} X_j^{0\sigma} + h.c.$$

$$+ \frac{J}{N} \sum_{ij} \epsilon_{\sigma\sigma'} \epsilon_{\eta\eta'} X^{\sigma\eta'} X^{\sigma'\eta} - \mu \sum_i X_i^{\sigma\sigma}, \quad (29)$$

where the summation over the Sp(2N) indexes $\sigma, \eta = \pm 1, \pm 2, ..., \pm N$ is assumed and the Sp(2N) antisymmetric tensor $\epsilon_{\sigma\sigma'} = \mathrm{sgn}(\sigma)\delta_{\sigma,-\sigma'}$. The local constraint of the t–J model can now be taken in the form $\sum_\sigma X_i^{\sigma\sigma} = N$ at every lattice site.

The exchange term in (29) can be rewritten in terms of the Sp(2N) invariant valence - bond operators $\tilde{B}_{ij}^+ := \sum_{\sigma\sigma'} \epsilon_{\sigma\sigma'} X_i^{\sigma 0} X_j^{\sigma' 0}$ in the form

$$-\frac{J}{N} \sum_{ij} \tilde{B}_{ij}^+ \tilde{B}_{ij}$$

and may be decoupled by the link field

$$\tilde{\Delta}_{ij} := \frac{1}{N} < \sum_{\sigma\sigma'} \epsilon_{\sigma\sigma'} X_i^{\sigma 0} X_j^{\sigma' 0} > .$$

At $N = \infty$ this decoupling becomes exact.

The su(2|1) supersymmetric representation of the Hubbard operators can be extended to the case of the su(2N|1) superalgebra. Since Sp(2N)⊂ SU(2N) one can then employ the su(2N|1) coherent states and the corresponding path integral to treat the t-J Hamiltonian (29). In this way we will eventually arrive at an Sp(2N) globally invariant generalization of the representation (23), with $\vec{S}$ and $\vec{M}$ operators being now replaced by the corresponding Sp(2N) generators. More details will be given elsewhere.

VII. CONCLUSION

To conclude we developed a RVB mean field theory which takes a direct account of the dopant carriers. These dopant particles are represented by appropriate fermion fields which carry both spin and charge and transform themselves as true SU(2) spinors. The resulting theory is written in a very convenient form since we are able in this way to consider the both doping dependence of the critical temperature as well as the kinetic energy effects which eventually destroy the superconductivity at larger dopings. By making a more extensive use of Hubbard operators we go beyond the conventional slave-boson approximation and take sufficient care of all symmetry properties of the Hamiltonian model. Since we apply a mean–field decoupling, there is always a gap in the energy spectrum of the dopant particles whenever $\Delta \neq 0$. Consequently, the superconducting transition temperature kT_c and the energy gap $J\Delta$ are of the same order. In the slave–boson RVB formulation of Ref. 6, for low doping T_c corresponds to the condensation of holons. Therefore, in that approach T_c is decoupled from the value of Δ. Such a decoupling may also occur within our approach, e.g., when spinons are considered beyond the mean–field level. One can see from Eq. (30) that the lowest–order spinon–holon coupling takes on the form $\frac{J\Delta}{2} \sum_{ij} \xi_i \xi_j (\bar{z}_j - \bar{z}_i) + h.c.$. The resulting density of states for holons may be finite also for $\Delta \neq 0$.[32]

We initially applied this new RVB scheme to describe the superconducting properties observed in the cobaltates. We succeeded in getting qualitative good agreement with experiment. The dome structure of the phase diagram $T_c \times \delta$ is well reproduced within a RVB framework[33]. This is achieved without any symmetry violation of the t-J model for the whole doping regime.

While preparing this version of our work we came across another RVB formulation in terms of dopant carriers[34]. Those authors use an extended t-J model with t, t' and t'' hopping parameters. In their scheme however those parameters are renormalized by interactions

and this procedure automatically violates the underlying symmetries of the original t-J model.

As discussed in the Appendix, the MF phase diagram $T_c(\delta)$ for the t-J model on the square lattice without frustration results in a max T_c located at $\delta = 1/2$. Although incorporating the next-nearest-neighbor (NNN) interaction in the kinetic term slightly shifts the diagram toward the origin, it cannot account for the experimentally observed curve for the cuprates. It's clear that frustration is an important ingredient for the success of our RVB method. However, apart from that there is yet another important feature with needs to be taken into consideration to properly deal with the cuprates case. In the cuprates there are strong antiferromagnetic correlations which manifest themselves even inside the superconducting vortex cores. As a result the $< \vec{S}_i \vec{M}_j >$ correlations, which seem unimportant for the cobaltates, may also play an important role in the cuprates.[35] This will produce strong phase fluctuations which, most likely, need to be taken into account beyond mean field approximation. This work is in progress and will be presented elsewhere.

As a final concluding remark let us say a few words about the ideology of the present paper. The basic idea is to use Hubbard operators, instead of the standard fermion operators accompanied with the nonholonomic constraint of no double occupancy. This enables us to impose the NDO constraint locally at each lattice site. This constraint results in strong electron correlation effects which are believed to be essential ingredients for dopped Mott insulators. Since the Hubbard operators appear as Gutzwiller projected (GP) electron operators on the states with no double occupancy, it is in principle reasonable to work directly with the GP operators and wave functions. In this way Paramekanti, Randeria and Trivedi recently studied the Hubbard model making use of parameters relevant for the cuprates, in the framework of the variational Monter Carlo GP d-wave state[36]. They showed that the strong electron correlations imposed by the Gutzwiller projection destroy the off diagonal long range order as $\delta \to 0$ qualitatively tracking the observed nonmonotonic $T_c(\delta)$. Basically the same result follows from the Plain Vanilla version of RVB, where the Gutzwiller projection is treated within the mean-field representation.

In our approach we also treat the NDO constraint at the mean-field level. However, we go a step further since we make explicit use of the algebraic relations between the Hubbard operators, namely those of the su(2|1) superalgebra. This adds some extra information which is encoded in the superalgebra commutation relations. In particular the classical phase space realization (the coherent-state representation) of su(2|1) provides us with the complex canonical coordinates (z, ξ) which eventually appear as the basic spinon-fermion fields in the path integral effective action (4). Dopant quasiparticle amplitudes (18) are constructed out of these fields appearing in our theory as emergent phenomena. We arrive naturally

in this way at the RVB theory for dopant carriers.

VIII. APPENDIX

In this Appendix we show that within the BCS MF approximation (28) the equations for the order parameter and the chemical potential are invariant under the change $t \to -t$, $\delta \to 1 - \delta$, $\mu \to -\mu$, provided the NDO constraint is rigorously taken into account.

First, we integrate out the fields $\Psi_{\uparrow i}, \overline{\Psi}_{\uparrow i}$ in Eq. (20) with the Hamiltonian function given by (28), which results in the effective action (15) with the classical Hamiltonian function now being,

$$H_{SC}^{cl} = -t\sum_{ij}(\xi_i\overline{\xi}_j\langle z_i|z_j\rangle + h.c.) - \mu\left(N - \sum_i \bar{\xi}_i\xi_i\right)$$
$$+\frac{J\Delta}{2}\sum_{ij}\left(\xi_i\xi_j\frac{\bar{z}_j - \bar{z}_i}{\sqrt{(1+|z_i|^2)(1+|z_j|^2)}} + h.c\right). \quad (30)$$

Here $z_i(t)$ and $\xi_i(t)$ are dynamical fields. This representation rigorously incorporates the constraint of no double occupancy. Because of the rather complicated form of the action, we are in general unable to write out explicitly a quantum counterpart of Hamiltonian (30) as a function of the su(2) spin generators and spinless U(1) fermionic operators. However, in the SC phase we get $z_i(t) = z_i$, which means that quantum fluctuations of the background spinon fields are ignored. In that case only the fermionic kinetic term is left in the action (15), and the quantum Hamiltonian can be easily identified,

$$H_{SC} = -t\sum_{ij}(f_i f_j^\dagger\langle z_i|z_j\rangle + h.c.) - \mu\left(N - \sum_i f_i^\dagger f_i\right)$$
$$+\frac{J\Delta}{2}\sum_{ij}\left(f_i f_j\frac{\bar{z}_j - \bar{z}_i}{\sqrt{(1+|z_i|^2)(1+|z_j|^2)}} + h.c\right). \quad (31)$$

The f_i's stand for the on-site spinless fermionic operators, with $\{f_i, f_j^\dagger\} = \delta_{ij}$ that correspond to the classical Grassmann amplitudes, $f^{cl} =: \xi$, which give $\{\xi_i, \bar{\xi}_j\} = 0$. The dynamical spinon field $z_i(t)$ looses its time-dependence and turns itself therefore into a sort of external classical c-valued spinon field.

Next, we evaluate the on-site free energy function,

$$F/N = -\frac{1}{N}Tr\, e^{-\beta H_{SC}}, \quad (32)$$

where the symbol Tr is used to indicate the summation over the fermionic degrees of freedom as well as the complex c-valued spinon fields:

$$Tr\,(\cdots) := \int D\mu_{su(2)}(\bar{z}, z)\, tr_{f,f^\dagger}\,(\cdots) \quad (33)$$

The z-integral in (33) appears as an ordinary multiple integral. In this way the order parameter and chemical potential are determined by the conditions $\partial F/\partial \Delta = 0$, $\partial F/\partial \mu = \delta - 1$ which explicitly give

$$\left\langle \frac{J}{2}\sum_{ij} f_i f_j \frac{\bar{z}_j - \bar{z}_i}{\sqrt{(1+|z_i|^2)(1+|z_j|^2)}} + h.c \right\rangle = 0, \quad (34)$$

and

$$\left\langle \frac{1}{N}\sum_i f_i^\dagger f_i \right\rangle = \delta, \quad (35)$$

respectively. Here $\langle(\cdots)\rangle := Tr\,(\cdots)e^{-\beta H_{SC}}/Tr\, e^{-\beta H_{SC}}$. It can be checked straightforwardly that eqs. (34) and (35) are invariant under the change $t \to -t$, $\mu \to -\mu$, $\delta \to 1 - \delta$. To see this one should simultaneously make the canonical transformation, $f_i \to f_i^\dagger$, and change the integration variables, $z_i \to -\bar{z}_i$. Accordingly, the phase diagrams $T_c(\delta)$ at $t > 0$ and $t < 0$ are located symmetrically with respect to the point $\delta = 1/2$.

Explicitly, the equations for the order parameter and chemical potential read

$$\frac{1}{N}\sum_{\vec{k}\in BZ} \frac{\tanh(\frac{E_{\vec{k}}\beta}{2})}{E_{\vec{k}}}\,|\,\beta_{\vec{k}}\,|^2 = \frac{Z}{J}, \quad (36)$$

$$\frac{1}{2N}\sum_{\vec{k}\in BZ} \frac{\tanh(\frac{E_{\vec{k}}\beta}{2})}{E_{\vec{k}}}(t_{\vec{k}} - \mu) = \delta - 1/2, \quad (37)$$

where

$$E_{\vec{k}}^2 = (t_{\vec{k}} - \mu)^2 + J^2\Delta^2\,|\,\beta_{\vec{k}}\,|^2, \quad (38)$$

and $t_{\vec{k}} = -2t\gamma_{\vec{k}}$, $\gamma_{\vec{k}} = \sum_{\vec{n}} \cos \vec{k}\vec{n}$. In the case of the 2D square lattice $\gamma_{\vec{k}} = \cos k_x + \cos k_y$, whereas $\gamma_{\vec{k}} = \cos k_x + 2\cos(k_x/2)\cos(k_y\sqrt{3}/2)$ for the 2D triangular lattice. For the $d_{x^2-y^2}$ pairing on the square lattice the phase factor reads $\beta_{\vec{k}} = \cos k_x - \cos k_y$. For the triangular lattice we assume a $d_1 + id_2$ symmetry of the order parameter.[4,5] Then,

$$\beta_{\vec{k}} = \cos k_x - \cos\frac{k_x}{2}\cos\frac{k_y\sqrt{3}}{2} + i\sqrt{3}\sin\frac{k_x}{2}\sin\frac{k_y\sqrt{3}}{2}. \quad (39)$$

The equations (36) and (37) are clearly seen to be invariant under the change $t \to -t$, $\mu \to -\mu$, $\delta \to 1 - \delta$, which results in the phase diagram depicted on Fig.1.

Note that the t-J Hamiltonian on a square lattice with the nearest-neighbor (NN) interaction is invariant under the change, $t \rightarrow -t$. This is because this change amounts to a certain unitary transformation of the lattice electron operators. It then follows that the above two phase diagrams merge in this case into one, located at $\delta = 1/2$. Incorporating frustration (e.g., by taking into account the NNN interaction in the t-dependent term) destroys this symmetry and results in splitting of this diagram again into two located symmetrically with respect to the point $\delta = 1/2$. However for the generic values of the t-J parameters that splitting is rather small and cannot account for an experimentally observed phase diagram for the cuprates.

If we ignored completely the NDO constraint taking into account the modes $\Sigma_{\vec{k}, \varpi_n > 0}$ and $\Sigma_{\vec{k}, \varpi_n < 0}$ on equal grounds, we would get (on a square lattice) a diagram with max T_c located at $\delta = 1$. This is markedly different from the NDO constraint-free BZA result, where max T_c occurs at $\delta = 0$, which bears out that our theory is in a sense dual to the original BZA approach.

The conventional BZA MF theory formulated in terms of the lattice electron spin singlets with the renormalization $t \rightarrow \delta t$ being implemented to partly incorporate the NDO constraint, however fails to maintain the symmetry of the phase diagram dictated by this constraint, and results in the same observation: max T_c takes place again

at $\delta = 0$, as in the constraint-free BZA theory. To see this consider the BZA MF Hamiltonian,[9]

$$H_{t-J}^{BZA} = -t\delta \sum_{ij\sigma} c_{i\sigma}^{+} c_{j\sigma} + h.c - \mu \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma}$$

$$+ \frac{J\Delta}{2} \sum_{ij} (c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow} + h.c.) + \frac{JNZ|\Delta|^2}{4}. \quad (40)$$

One obtains the following system of equations to determine the order parameter and chemical potential:

$$\frac{1}{N} \sum_{\vec{k}} \frac{\tanh(\frac{E_{\vec{k}}\beta}{2})}{E_{\vec{k}}} \gamma_{\vec{k}}^2 = \frac{Z}{2J}, \quad (41)$$

$$\frac{1}{N} \sum_{\vec{k}} \frac{\tanh(\frac{E_{\vec{k}}\beta}{2})}{E_{\vec{k}}} (t_{\vec{k}} - \mu) = \delta, \quad (42)$$

where

$$E_{\vec{k}}^2 = (t_{\vec{k}} - \mu)^2 + J^2 \Delta^2 \gamma_{\vec{k}}^2, \quad (43)$$

and $t_{\vec{k}} = -2t\delta\gamma_{\vec{k}}$, $\gamma_{\vec{k}} = \sum_{\vec{n}} \cos \vec{k}\vec{n}$. The ensuing phase diagram $T_c^{BZA}(\delta)$ is invariant under the change $\delta \rightarrow -\delta$ so that max T_c always occurs at $\delta = 0$.

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